STRUCTURE AND BONDING OF DIBROMINE MONOXIDE, Br_2O, IN THE GAS PHASE

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The rotational spectrum of the unstable Br_2O molecule has been studied for the first time in selected regions between 90 and 523 GHz in the ground vibrational state for the $^{79}Br_2O$, $^{79/81}Br_2O$, and $^{81}Br_2O$ isotopomers. The first excited bending mode has been investigated for the mixed isotopomer. The spectrum is that of a near symmetric prolate rotor ($\kappa \approx -0.9966$) with the dipole moment along the b-axis. The combination of a relatively large A rotational constants along with small values for B and C give rise to a large range of J (6 - 123) and K_a quantum numbers (0 - 12) observed in the spectral regions. Rotational, centrifugal distortion, nuclear quadrupole and spin-rotation coupling constants have been determined, as well as centrifugal distortion terms for the quadrupole constants. Quadrupole splittings are large and can be observed for lines above J = 0. The diagonalization of the quadrupole tensor indicates a rather covalent Br-O bond. The molecular structure and the harmonic force field have been derived and are compared with data for related molecules.